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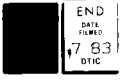

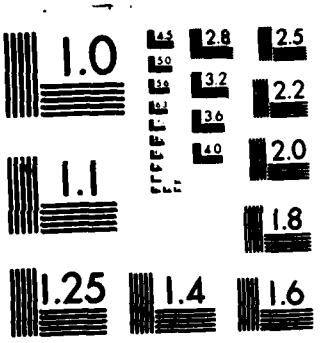

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Biological Water; Diffusion; Neutron Scattering; Brine Shrimp Artemia

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The method of quasi-elastic neutron scattering was used to study the properties of water associated with macromolecular systems. We determined the diffusion parameters for pure water, agarose gel (4 gm H_2O/gm dry solids). The scattering has been interpreted with a scattering law derived from a jump-diffusion model for the translational motion and a Brownian diffusion model for the rotational motion. Results were obtained for the

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neutron line width Γ as a function of the momentum change of the scattered neutron, $\hbar Q$. From $\Gamma(Q)$, we obtain the parameters of the models that characterize the diffusion. We find that the diffusive motion for the water in the agarose gel is restricted by its association with the polymer molecules, the diffusion coefficient being reduced from that of pure water by ~20%. The properties of the water in the Artemia cysts differ greatly from those of pure water. The translational diffusion coefficient is reduced by a factor of ~4 and the rotational diffusion coefficient by ~13. These changes are an intrinsic property of the cyst water produced by its association with the bio-polymers.

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FINAL REPORT NO. F1

The Measurement of the Diffusive Motion of Protons in Biological Systems

by

H. E. Rorschach, Jr.

W. M. Rice University
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Houston, TX 77251

2 June 1983

Index

I. Summary of Research Accomplishments

The principal investigator of this project, with funding from the Office of Naval Research, has initiated a series of neutron scattering studies during the last 4 years which were intended to test the applicability of the method of quasi-elastic neutron scattering (QNS) to the study of water in macromolecular systems, especially biological systems. These studies were carried out in collaboration with Dr. R. M. Nicklow at Oak Ridge National Laboratory (ORNL), Dr. C. F. Hazlewood of the Baylor College of Medicine, Professor J. S. Clegg of the University of Miami, and E. C. Trantham and D. B. Heidorn, graduate students in the Physics Department at Rice University. We have conducted our studies on the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory, utilizing a triple-axis spectrometer to perform the first QNS studies ever conducted in that laboratory.

Our studies, reported in detail in the references indexed in Section II were designed to answer three experimental questions:

1. Is the resolution of the Oak Ridge spectrometer sufficient to do QNS studies?
2. Can the scattering from the water protons be separated from that due to the macromolecular protons?

3. Can a biological system of some significance remain viable for the time (~1 week) needed to obtain the complete QNS spectra in (ω,Q) space?

Our experiments on water, gels of agarose and polyox, and the cysts of the brine shrimp (Artemia) gave an affirmative answer to these questions.

Our first experiments were on pure water. The spectra were in good agreement with those obtained by other investigators, and we were able to obtain good values for the parameters that describe the diffusive motion (e.g. the diffusion coefficient D and the residence time τ in a jump-diffusion model). The resolution of the ORNL spectrometer was adequate for our purposes. Experiments on agarose and polyox-H_2O gels, containing known amounts of covalently bonded protons, showed that a two-component model (an elastic and an inelastic component) gives a good approximation to the scattering law. The fraction of the scattering due to each component could be obtained from an analysis of the spectra combined with studies of D_2O gels of these polymers.

Our most exciting results were obtained on the Artemia cysts. This system is an important biological model, and is especially suited for QNS studies, since the hydration of the cysts can be varied over a wide range (~0-1.4 grams H_2O/grams

dry solids) without affecting the viability of the cysts. The viability is unaffected by long exposure (~1 week) to neutrons, which permits the extended experiments necessary to obtain a complete spectral scan on the HFIR triple-axis spectrometers. Our results show that the neutron spectra are not consistent with the assumption that the water in the cyst is "free," but that the translational and rotational diffusion coefficients are substantially reduced from the values for pure water. These reductions are an intrinsic property of the water in the cyst and cannot be ascribed to interaction with barriers or obstructions. The neutron scattering results can be shown to be consistent with NMR and dielectric relaxation studies, so that we have a promising beginning for the development of a comprehensive model that unifies the results of several measuring methods.

II. Index of Technical Reports and Publications

A. Technical Reports: NONE

B. Publications*:

1. Trantham, C., H. Rorschach, R. Nicklow and N. Wakabayashi. "Quasi-Elastic Neutron Scattering for the Agarose-Gel System." Proc. Fed. Am. Soc. Exp. Biol. 39 (1980) 1958.

2. Trantham, E. C., H. E. Rorschach, J. C. Clegg, C. F. Hazlewood and R. M. Nicklow. "QNS Measurements on Water in Biological and Model Systems." in Neutron Scattering - 1981, AIP Conference Proceedings No. 89. Ed. John Faber, Jr. (AIP, New York, 1982) pp. 264-266.

3. Trantham, E. C., Rorschach, H. E., Clegg, J. S., Hazlewood, C. F., Nicklow, R. M., and Wakabayashi, N. "The Diffusive Properties of Water in Artemia Cysts as Determined from Quasi-Elastic Neutron Scattering Spectra," Biophysical Journal, submitted.

4. Rorschach, H. E., Trantham, E. C., Heidorn, D. B., Hazlewood, C. F., Clegg, J. S., Nicklow, R. M., and Wakabayashi, N. "The Diffusive Motion of Protons in Pure Water, Agarose Gel and Artemia Cysts as Measured by Quasi-Elastic Neutron Scattering," Proceedings of the U.S.-Romania Workshop on New Trends in the Study of Water and Ions in Biological Systems, Romanian Press, in press.

5. Rorschach, H. E. "Water in Polymers and Artemia Cysts: Relation of Neutron Scattering and NMR Results," Proceedings of the Second International Conference on Water and Ions, Plenum Press, in press.

*Preprints/reprints of these manuscripts are available from the principal investigator on request.

III. Conclusions of Research

- The technique of quasi-elastic neutron scattering (QNS) can be fruitfully applied to study the dynamics of water in carefully chosen polymer and biological systems. It yields new information complementary to that obtained by other methods.
- The triple axis spectrometers at the HFIR reactor at ORNL are suitable for QNS studies on biological systems for momentum transfers $\hbar Q$ in the range $0.5\ A^{-1} < Q < 3\ A^{-1}$.
- The dynamical properties of water in gels of agarose and poly(ethylene) oxide and in cysts of the brine shrimp (Artemia) have been studied with QNS. In all of these systems, the diffusive properties of water differ significantly from those of pure water. The changes are especially dramatic for the Artemia cysts and show that nearly all of the water in this system has greatly reduced translational and rotational diffusion coefficients.

IV. Major Accomplishments

- The application of the QNS technique to the study of water in viable biological systems is new, and we have shown that this technique has great potential for future studies.
- Data analysis methods for the reduction of neutron scattering data and the analysis of multiple scattering from heterogeneous biological systems have been developed.
- A model biological system (cysts of Artemia) has been identified that combines biological importance with the characteristics needed for QNS studies (viability and accessible hydration range).
- A major paper on this work has been prepared and submitted for publication to the Biophysical Journal (see Section IIB. item 3).

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